3-Methylindene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.52e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.01e-01

Confidence level: 6.48e-01

Nearest Neighbors from the Training Set

Image not found
2,4-Dichloro-1-(chloromethyl)benzene
Measured: 1.10
Predicted: 1.19e-01

Image not found
Benzophenone
Measured: 3.68e-01
Predicted: 7.04e-04

Image not found
alpha-d-glucopyranose
Measured: 1.47
Predicted: 3.93e-13

Image not found
Carbophenothion
Measured: 3.99e-02
Predicted: 4.02e-07

Image not found
2,6-Dimethylpyridine
Measured: 5.79e-01
Predicted: 1.35